

Some Fundamental Physical Properties of BiGaO₃ Cubic Perovskite

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Abstract : Some fundamental physical properties of BiGaO₃ were investigated under pressure and temperature effect using generalized gradient approximation and local density approximation approaches. The effect of orientation on Debye temperature and sound waves velocities were estimated from elastic constants. The value of the bulk modulus of BiGaO₃ is a sign of its high hardness because it is linked to an isotropic deformation. BiGaO₃ is a semiconductor and ductile material with covalent bonding (Ga-O), and the Bi-O bonding is ionic. The optical transitions were observed when electrons pass from the top of the valence band (O-2p) to the bottom of the conduction band (Ga-4p or Bi-6p). The thermodynamic parameters are determined in temperature and pressure ranging from 0 to 1800 K and 0 to 50 GPa.

Keywords : BiGaO₃ perovskite, optical absorption, first principle, band structure

Conference Title : ICCEPS 2022 : International Conference on Chemical Engineering and Physical Sciences

Conference Location : Istanbul, Türkiye

Conference Dates : December 20-21, 2022